

Asymmetrical Inter-Symbol Interference in Macro-Scale Molecular Communications

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ABSTRACT

Molecular communication (MC) is new method of information transmission whereby information is carried by chemical signals instead of electromagnetic (EM) waves. This shift to a new type of information carrier makes MC a viable option in circumstances where EM communication might prove inefficient, e.g., in underwater and underground communications or for in-body and biological applications. To date, almost all MC systems that have been proposed have focused on nano- and micro-scale communications, however recent research has sought to implement MC at macro-scales. A major problem of MC is the inter-symbol interference (ISI) caused by residual chemicals leftover from a previous transmission which can cause incorrect decoding of the signal. This paper reports an experimental study conducted on transmitting MC at the macro-scale. A mass spectrometer (MS) was used as the detector and an algorithm was designed to help mitigate the memory effect of the channel. It is shown that by using the algorithm, communication in the macro-scale is made more practical and feasible.

KEYWORDS

Inter-symbol Interference, Molecular Communications, Mass Spectrometer.

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1 INTRODUCTION

The transmission of information is a well-understood process and for over a century, information transmission has been conducted

using EM waves. Even though EM communication systems have achieved numerous feats, there are shortcomings in some areas where an alternative system might be a better option. For example, areas with limited spectrum availability or with environments with high EM absorption rates [20]. As a result of these drawbacks, MC offers an alternative mode of communication [1, 15, 17]. MC uses chemical particles (atoms and molecules) as information carriers. Such methods are widely utilized in nature (e.g. pheromones etc.). There have been studies done in various aspects of MC including modulation [8, 9] error correction [10, 11] and channel capacity [2, 12, 16]. However, most studies in the field have been done at the micro-scale (nm - μ m). In addition to theoretical studies a few practical applications have been tested [5] that have shown the feasibility of MC use at macro-scale (cm - m) [7] levels.

A problem in macro-scale MC is that following the propagation of the chemical signal leftover chemicals from a previous message transmission can cause inter-symbol interference (ISI) [13, 19, 21]. To overcome this, there are two options that can be used. The first is to increase the bit duration of the transmission. However, this will decrease the transmission speed of an already slow system. The second option, which is the topic of discussion in this paper, utilizes an algorithm that can adapt to the changing signal patterns of a MC transmission.

In this paper experimental tests were conducted on the reliability and feasibility of a macro-scale MC. For the transmitter, a custom-built odor generator [6] is used and for the detector a quadrupole mass analyzer (QMA) is utilized, the details of which can be seen in Section 2. In section 3 the transmitted signal is analyzed and the ISI effects are shown, and an algorithm is described that mitigates the ISI on MC communications. Section 4 presents and discusses the results obtained.

2 EXPERIMENTAL SETUP

To realize the experiment, two devices were used. To transmit the chemicals based on a message, an in-house-built odor generator, and to detect the chemical a mass spectrometer (MS) with a quadrupole mass analyzer (QMA) were used. A MS is an analytical tool that can analyze and distinguish chemicals in a given sample. The transmitter side of the experimental setup is shown in Figure 1, the detector shown in Figure 3 and the details of both the transmitter and the receiver are given below.

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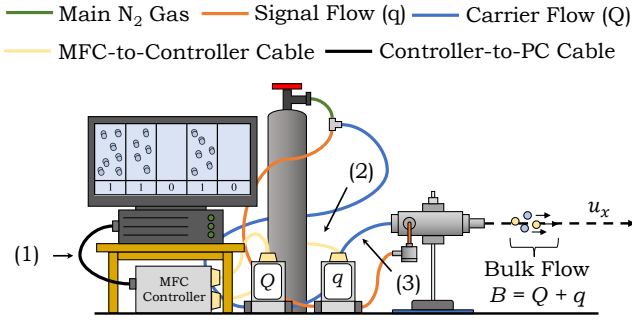


Figure 1: Diagram of the Transmitter Setup: (1) Modulation information is carried to the MFC Controller (2) From the controller the pulses are sent to MFC's where they are converted into gas pulses (3) These pulses are carried into the mixing chamber (Q) and the evaporation chamber (q).

2.0.1 Transmitter. The transmitter is a controlled gas dispenser that releases the evaporative chemicals in an evaporation chamber along with a carrier gas (N_2) based on mass flow controllers (MFC) that manage the flow for both the carrier and the signal gases [18]. The inlet for the evaporation chambers has a thermo-resistant septum that lets the user inject chemicals directly into the evaporation chamber multiple times [6]. The diagram of the transmitter and its mechanism can be seen in Figure 2.

There are 3 types of flows present in the transmission of chemicals (acetone, methanol and nitrogen). The first one is the signal flow (q) where a small amount of N_2 gas ($q \ll Q$) is used to carry the sample in the evaporation chamber into the mixing chamber. The second one is the carrier flow where the majority of the N_2 is used to carry the chemicals from the mixing chamber into the transmission medium. When both the signal chemicals and the carrier chemicals are in the medium, it is defined as bulk flow (B).

2.0.2 Chemicals. In this experiment three chemicals (acetone, methanol and nitrogen) were used. The carrier gas (Q) was chosen as zero-grade N_2 (% 99.998 purity). The signal gas (q) was acetone (% 99.8 purity) which was diluted in methanol (over % 99.9 purity). Acetone was diluted in methanol to produce a 1-part acetone 10-part methanol solution. This was done to avoid the over-saturation of the MS membrane.

2.0.3 Detector. A portable membrane inlet mass spectrometer (MIMS), Provided by Q Technologies Ltd., was used in the experiment. The inlet of the system possesses a fine non-sterile flat polydimethylsiloxane membrane [6]. The membrane in the system acts as a filter and diminishes random fluctuations and the noise detected. This improves the signal-to-noise ratio (SNR); however, the existence of the membrane causes delays in the retrieval of the transmitted signal. A detailed diagram of the detector can be seen in Figure 3.

More detailed information regarding the setup can be seen in [6], and the parameters of the experiment can be seen in Table 1. On-Off Keying (OOK) is defined such that the presence of the signal chemical with the addition of the carrier flow is defined as 1 ($Q +$

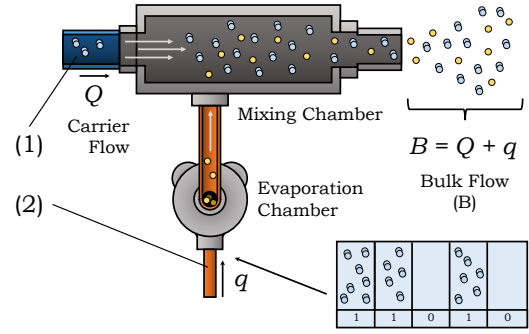


Figure 2: Transmitter Mechanism (Odor Generator): (1) The carrier flow rate (Q) is controlled by a MFC which is directly connected to a N_2 tank, The carrier flow carries the chemicals from the mixing chamber to the transmission medium. (2) The signal flow rate is controlled by a MFC which is directly connected to a N_2 tank. The signal flow carries the chemicals from the evaporation chamber to the mixing chamber

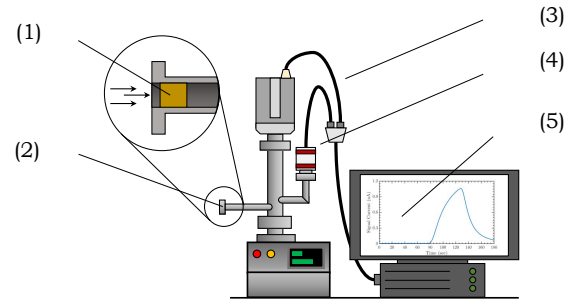


Figure 3: A diagram of the detector: (1) Semi-permeable membrane (2) Detector inlet (3) Retrieved ion Data (4) MS Vacuum Pressure controller (5) Single-ion Monitoring.

Table 1: Experiment Parameters

Property	Symbol	Quantity	Unit
Transmission distance	x	2.5	cm
Signal flow	q	8	ml/min
Carrier flow	Q	750	ml/min
Bit duration	t	20	s

q) and the absence of the signal chemical is defined as 0 (Q). The carrier gas (Q) is kept at a constant value for both 0 bit and 1 bit transmission with a value of 750 ml/min.

3 TRANSMISSION OF INFORMATION

Any communication based on particles or molecules with flow present can be modelled by a simplified version of the advection-diffusion equation [3, 4]. By assuming that there is only flow in the x-direction, with zero divergence, and there are no sources or sinks in the system and the diffusivity coefficient is constant, the advection-diffusion equation for 1-D can be written as;

$$\frac{\partial C(x, t)}{\partial t} = D \frac{\partial^2 C(x, t)}{\partial x^2} - u_x \frac{\partial C(x, t)}{\partial x} \quad (1)$$

The solution of this equation with an instantaneous and localized release ($C(x = 0, t = 0) = M\delta(x)$) is:

$$C(x, t) = \frac{A}{\sqrt{t}} \exp \left[-\frac{(x - u_x t)^2}{4Dt} \right] \quad (2)$$

Where D is the coefficient of diffusivity (m^2/s), t is the time (s), u_x is the 1-D flow in the x-axis (m/s) and C is the concentration of the chemicals in 1-D (mol/m or gr/m). A is a constant of the equation which can be shown as;

$$A = \frac{q}{\sqrt{4\pi D}} \quad (3)$$

Where q is the amount of chemical injected into the system (mol or gr). In Eq. (2), the exponential nature of the chemical concentration decay predicts that the system will retain chemicals, and this influences the next pulse. The time at which the detected concentration value reaches its maximum value the can be calculated as;

$$\frac{dC(x, t)}{dt} = -\frac{q(u_x^2 t^2 + 2Dt - x^2)}{8t\sqrt{\pi(Dt)^3}} \exp \left[-\frac{(x - u_x t)^2}{4Dt} \right] \quad (4)$$

$$t_{max} = \frac{\sqrt{u_x^2 x^2 + D^2} - D}{u_x^2} \quad (5)$$

Based on Eq. (5) it is shown that the time at which the concentration reaches the maximum is independent of the chemicals injected into the system. After the system reaches maximum concentration $C(x, t_{max})$ it starts to experience concentration decay. If the bit duration of the communication is set as T , the leftover concentration from the transmission can be expressed as,

$$C_{ISI} = \sum_{n=0}^{n=\infty} [C(x, nt + T) - C(x, nt)] \quad (6)$$

Depending on which bit was transmitted (0, 1) the values of ISI will be different. This is caused by the uneven time between the rise time and the fall time of the concentration function $C(x, t)$.

In an OOK communication there are four possible scenario, where leftover chemicals can be encountered. These are $C_{ISI_{00}}$, $C_{ISI_{01}}$, $C_{ISI_{11}}$ and $C_{ISI_{10}}$ where they represent the state transmission from 0 to 0, 0 to 1, 1 to 1 and 1 to 0 respectively.

$$C_{ISI} = \begin{bmatrix} C_{ISI_{10}} & C_{ISI_{11}} \\ C_{ISI_{00}} & C_{ISI_{01}} \end{bmatrix} \quad (7)$$

In order to calculate the probability of the total ISI in a transmission a Markovian process is used to model this behavior, as shown in Figure 4. The Markov chain process of the transmission is;

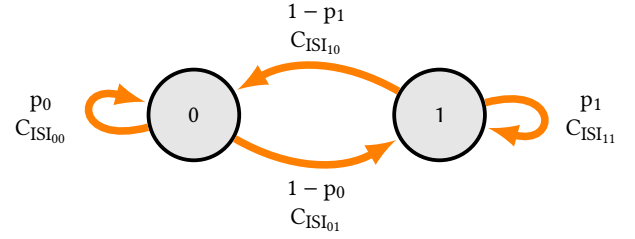


Figure 4: A Markov Chain Diagram

$$C_{ISI} = \begin{bmatrix} 1 - p_1 & p_1 \\ p_0 & 1 - p_0 \end{bmatrix} \quad (8)$$

Where if N number of bits are transmitted the steady state solution of the probability matrix given in Eq. (8) can be calculated as;

$$\lim_{m \rightarrow N} P^m = \begin{bmatrix} \frac{1-p_1}{[2-(p_0+p_1)]} & \frac{1-p_1}{[2-(p_0+p_1)]} \\ \frac{1-p_0}{[2-(p_0+p_1)]} & \frac{1-p_0}{[2-(p_0+p_1)]} \end{bmatrix} \quad (9)$$

Therefore, the total leftover accumulated chemicals that can cause ISI can be expressed as;

$$C_{ISI} = N (-P_{11}C_{ISI_{10}} + P_{12}C_{ISI_{11}} - P_{21}C_{ISI_{00}} + P_{22}C_{ISI_{01}}) \quad (10)$$

As it can be seen from Eq. (10), each transmission adds or removes chemicals to the system with $C_{ISI_{01}}$ and $C_{ISI_{11}}$ adding more chemicals to the system and $C_{ISI_{10}}$ and $C_{ISI_{00}}$ removing more chemicals from it. Based on the steady state matrix in Eq. (9), Eq. (10) can be rewritten as;

$$C_{ISI} = N \left[\frac{(1-p_1)(C_{ISI_{11}} - C_{ISI_{10}}) + (1-p_0)(C_{ISI_{01}} - C_{ISI_{00}})}{[2-(p_0+p_1)]} \right] \quad (11)$$

However, because the residue chemicals from each bit transmission may be different, for long transmission (i.e. $p_1 = p_0 = 0.5$) the system will accumulate more chemicals than it flushes.

$$C_{ISI} = \frac{N}{2} (C_{ISI_{01}} + C_{ISI_{11}} - C_{ISI_{10}} - C_{ISI_{00}}) > 0 \quad (12)$$

If there is a static threshold value defined as C_τ and both decoded 0 and 1 bits produce a Gaussian distribution of $X_0 \sim \mathcal{N}(\mu_0, \sigma_0^2)$ and $X_1 \sim \mathcal{N}(\mu_1, \sigma_1^2)$ the error rate that occurs because of ISI can be expressed as;

$$p(0|1) = \text{erfc} \left(-\frac{(\mu_0 + C_{ISI} + C_\tau)}{\sqrt{2}\sigma_0} \right) \quad (13)$$

$$p(1|0) = \text{erfc} \left(\frac{(\mu_1 + C_{ISI} + C_\tau)}{\sqrt{2}\sigma_1} \right) \quad (14)$$

$$p(0|1) > p(1|0) \quad (\sigma_1 \sim \sigma_0) \quad (15)$$

This in turn, increases the error of wrong decoding of 0 as 1 $p(0|1)$ at a higher rate than the wrong decoding of 1 as 0 $p(1|0)$, making the system behave as a binary asymmetric channel (BAC).

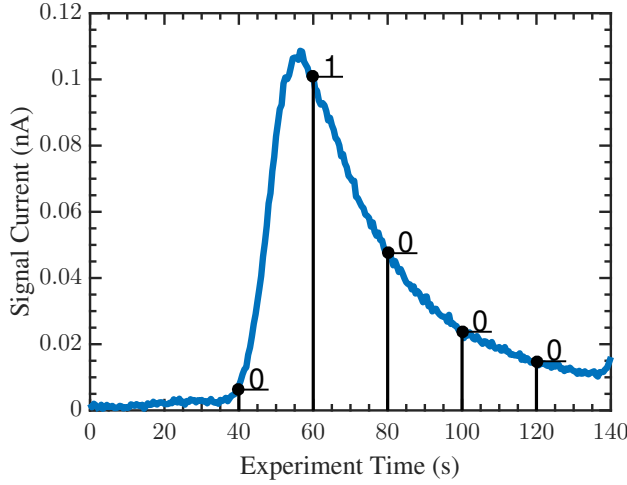


Figure 5: A sample of transmission of "01000"

3.1 ISI-Free Communication

To find the optimum zero-to-one ratio (z/o) that leaves no chemicals in the system, the integration of the concentration function is taken.

$$\int C(x, t) dt = \chi(x, t) \quad (16)$$

$$\chi(x, t) = \frac{q}{2u_x} \left(B_1 + \exp\left(\frac{u_x x}{D}\right) B_2 + 1 \right) + \text{constant} \quad (17)$$

Where

$$B_1 = \text{erf}\left(\frac{u_x t - x}{\sqrt{4Dt}}\right) \quad (18)$$

$$B_2 = \text{erf}\left(\frac{u_x t + x}{\sqrt{4Dt}}\right) - 1 \quad (19)$$

The steady-state value of the function is:

$$C = \lim_{t \rightarrow \infty} \chi(x, t) = \frac{q}{u_x} + \text{constant} \quad (20)$$

If the system is left long enough, the concentration of the transmitted chemicals reaches 0 ($\partial\chi/\partial t = 0$). If the sampling period defined as T and consecutive zeros are transmitted after one, the ratio of the amount of chemicals cleaned from the system to the chemicals given to the system approaches 1:

$$\lim_{n \rightarrow \infty} \left[\frac{C(x, t)}{C(x, t) - C(x, t + nT)} \right] = 1 \quad (21)$$

Therefore, to have a complete ISI-free system in our MC setup, a single 1 bit must be accompanied by an infinite number of 0's. However, in practice it is possible to trade BER performance against zero stuffing.

4 LINE CODING EXPERIMENT

One of the major problems of using molecules in transmission is the leftover from previous chemicals. Chemicals sensors, therefore need to be cleaned in order to overcome the problem of the memory effect. However, the sensor cleaning time can be long especially

with a membrane present in the detector, adding a further delay to the signal. In Figure 5 a stream of bits consisting of 01000 is shown. The transition from '0' to '1' is retrieved as expected. However, the 0's following the '1' show that the cleaning of chemicals at the detector is not fast enough. Additionally, each consecutive '0' flushes less chemicals than the previous '0' and in a communication where hundreds of bits are transmitted, this can cause a problem of decoding if a simple threshold mechanism is used. Moreover, because of the behaviour of molecular communications, the transmission time given for a single bit may not be enough for the signal to reach to the background noise level, e.g. if there is a single 0 between a string of '1's, the '0' bit produces a higher signal current than the background noise level at the beginning of the transmission (i.e. a single '0' cannot flush all the chemicals leftover from consecutive '1's). In addition, the next '1' bit adds additional chemicals (C_1) to the leftover chemicals (C_{ISI}) which in turn produces even higher signal current. Therefore, if there are more '1's than '0's present in the transmission this could lead to an increase of the overall signal amplitude, making a simple threshold detector inefficient at decoding the transmission correctly.

In our experimental transmission system, the signal current values (measured by the QMA) for the '1' bit ranges from 0.1 nA to 0.53 nA and '0' ranges from 0.37 nA to 0.006 nA. The overlaps between '0' values and '1' caused by the residual chemicals from the previous bit can cause incorrect decoding of the transmitted signal. To overcome this, instead of relying on the amplitude values of each bit, the behaviour of the bits relative to the previous bit was investigated

5 RESULTS

The properties of chemical transmission make the simple threshold detection inefficient because of varying amplitude values based on the residue chemicals from previous transmission, therefore a detection method based on relative bit value is better suited for this type of communication system. The mechanism of the algorithm is as follows;

The mechanism of the algorithm is as follows;

- (1) The initial bit is determined by a predefined threshold in which this experiment is defined as $\tau = 0.1$ nA.
- (2) The second bit is then defined relative to the previous decoded bit; if it is higher it is defined as 1, lower it is defined as 0.

To avoid errors due to unpredicted signal amplitude changes (e.g. due to fluctuations in the air, the following error correction routine was implemented:

- (3) Every retrieved signal data was compared to the previous one and if the difference is within a specified range it was defined as the previous bit. The range is calculated empirically since every chemical will react differently with the detector. For acetone, the range value coefficient assigned as $k = 0.1$.

The algorithm is shown below:

In our experiment, a message was sent in ASCII binary code. The message chosen was the first line from the novel Moby Dick 'Call me Ishmael' [14]. The message was converted to chemical data where bit '1' was assigned as a signal gas pulse of 8 ml/min and bit '0' was with no pulse; and both bits having a carrier flow of 750

Algorithm 1: Function Relative Bit Decoding (R, D)

Data: Retrieved signal values of the transmission array R

Result: Decoded values of the transmission array D

```

for n = 1 to length(R) do
  if n = 1 then
    if B(n) < τ then
      D(n) = 0
    else
      D(n) = 1
    end
  else if B(n) > B(n-1) then
    if |B(n-1) - B(n)| < kB(n) then
      D(n) = D(n-1)
    else
      D(n) = 1
    end
  else if B(n) < B(n-1) then
    if |B(n-1) - B(n)| < kB(n) then
      D(n) = D(n-1)
    else
      D(n) = 0
    end
  end
end
end

```

ml/min nitrogen gas was used. Using a static threshold value of $\tau = 0.191$ nA, 5 bits out of 120 transmitted were decoded incorrectly however, with the algorithm the decoding error value decreased to 1 bit in 120 bits. The errors occurred with the threshold detection is due to the changing amplitudes of '0's and '1's as the transmission evolves. The lower errors in the relative bit decoding shows that the algorithm is better at decoding a molecular message than threshold detection.

5.1 Bit Error Rate (BER)

To model the above system, two types of interference were considered. One was the background noise (σ_N^2) being detected by the receiver, (lingering chemicals in the atmosphere, leftover molecules from the previous transmission etc.) and the ISI effect (σ_{ISI}^2) caused by leftover chemicals. To model the background noise, Additive White Gaussian Noise (AWGN) with a distribution of $\mathcal{N}(\mu_N, \sigma_N^2)$ is used. The ISI is modelled with the μ_{ISI} being the intersection points of 1's and 0's distribution, $X_1 \sim \mathcal{N}(\mu_1, \sigma_1^2)$ and $X_0 \sim \mathcal{N}(\mu_0, \sigma_0^2)$ respectively, in the transmission.

$$\mu_{ISI} = \frac{\mu_0 \sigma_1^2 - \sigma_0 \left(\mu_1 \sigma_0 + \sigma_1 \sqrt{(\mu_1 - \mu_0)^2 + 2(\sigma_1^2 - \sigma_0^2) \log \frac{\sigma_1}{\sigma_0}} \right)}{(\sigma_1^2 - \sigma_0^2)} \quad (22)$$

The variance of the ISI (σ_{ISI}^2) is calculated using experimental values. The amplitude of the signal is calculated as the overall average amplitude of the '1' bits transmission and the total disturbance in the system is defined as;

Table 2: Example of a transmitted signal and decoded signal

Transmitted	0	1	0	1	0	1	0	0
Decoded	0	+1	-1	+1	-1	+1	-1	0

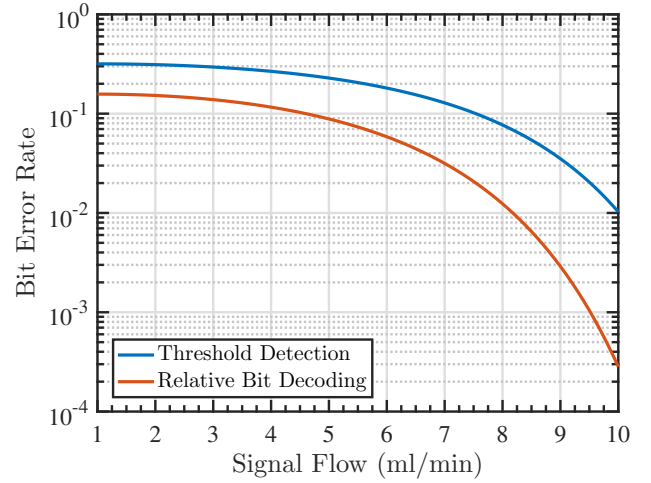


Figure 6: Comparison of BER values for threshold detection and Relative bit decoding

$$N = \sigma_N^2 + \sigma_{ISI}^2 \quad (23)$$

The bit error rate (P_e) for the simple threshold for equal probability of transmitting '1' and a '0' can be calculated as;

$$P_e = \text{erfc} \left(\sqrt{\frac{S}{2N}} \right) \quad (24)$$

Because of the way relative bit decoding (RBD) decodes a signal (As seen in table 2), the signal is converted into a polar signal.

The bit error rate therefore, for this method therefore can be expressed as:

$$P_e = \text{erfc} \left(\sqrt{\frac{S}{N}} \right) \quad (25)$$

The BER comparison of simple threshold detection and relative bit decoding can be seen in Figure 6

As it can be seen in Figure 6, the relative bit decoding performs better compared to threshold detection.

6 CONCLUSION

An experiment was conducted on the possibility of transmitting information using chemical odors as a means of macro-scale MC. A QMA was used as the detector and an in-house-built odor generator was used as a transmitter. It was shown that a molecular communication possesses an inter-symbol interference (ISI) effect due to the nature of chemical transmission and the presence of a membrane in the detector. An algorithm was devised to mitigate the effects of ISI. The algorithm, which is based on the bits value

relative to the previous ones, shows improved decoding compared to a simple threshold decoding. Finally, the Bit Error Rate of both types of decoding were compared.

In the future, improvements to the communication system will be studied along with the characteristic properties of molecular communications.

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